



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:43 PM UTC

PDB ID : 5Z0R / pdb_00005z0r
Title : Structural insight into the Zika virus capsid encapsulating the viral genome
Authors : Li, T.; Zhao, Q.; Yang, X.; Chen, C.; Yang, K.; Wu, C.; Zhang, T.; Duan, Y.;
Xue, X.; Mi, K.; Ji, X.; Wang, Z.; Yang, H.
Deposited on : 2017-12-20
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

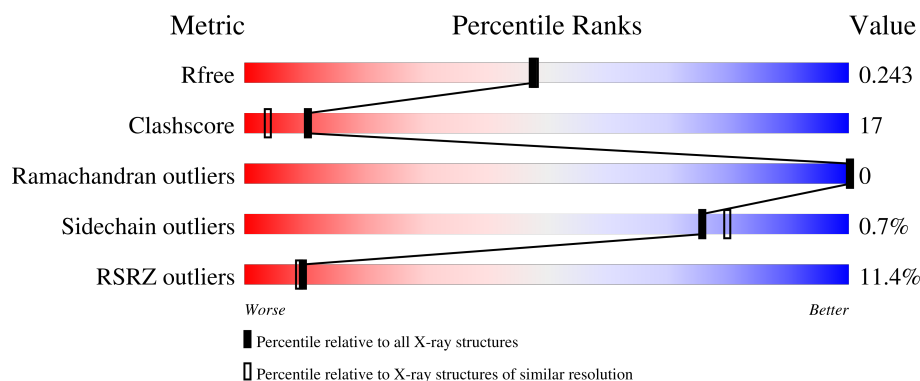
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	445	18% 68% 31% .
1	B	445	5% 74% 26%
2	C	2	100%
2	D	2	50% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7342 atoms, of which 44 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Extracellular solute-binding protein family 1, viral genome protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3425	2215	569	632	9			
1	B	445	Total	C	N	O	S	0	0	0
			3454	2234	573	637	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A140NCD0
A	268	ASP	ASN	engineered mutation	UNP A0A140NCD0
B	1	MET	-	initiating methionine	UNP A0A140NCD0
B	268	ASP	ASN	engineered mutation	UNP A0A140NCD0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			45	12	22	11			
2	D	2	Total	C	H	O	0	0	0
			45	12	22	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	154	Total	O	0	0
			154	154		

Continued on next page...

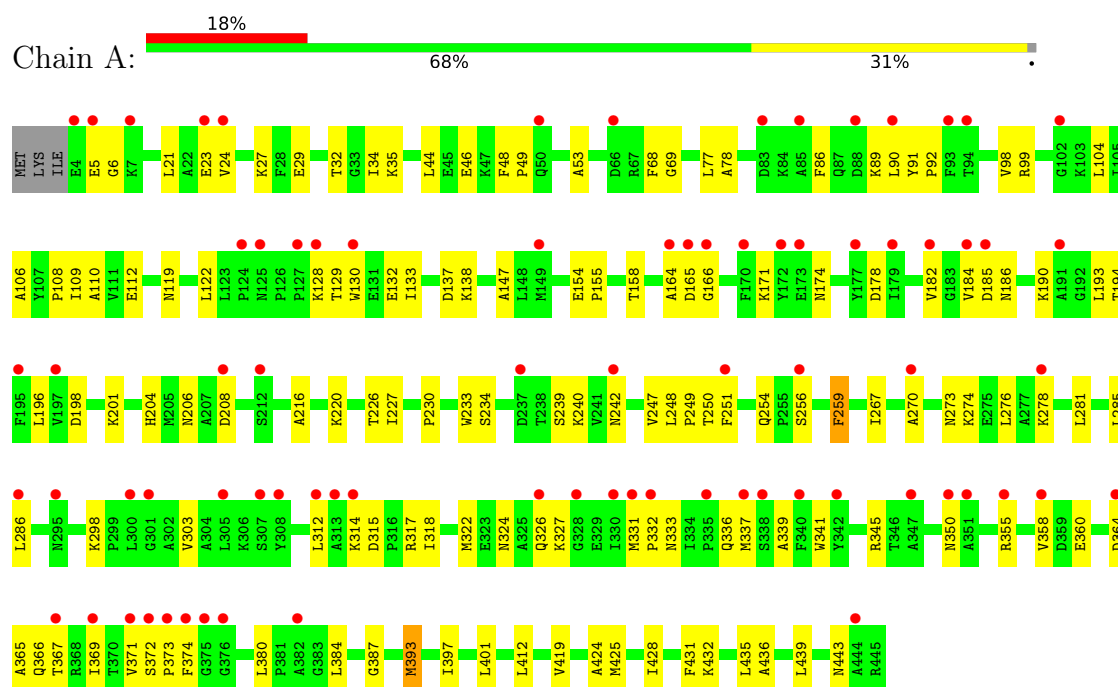
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	219	Total 219	O 219	0	0

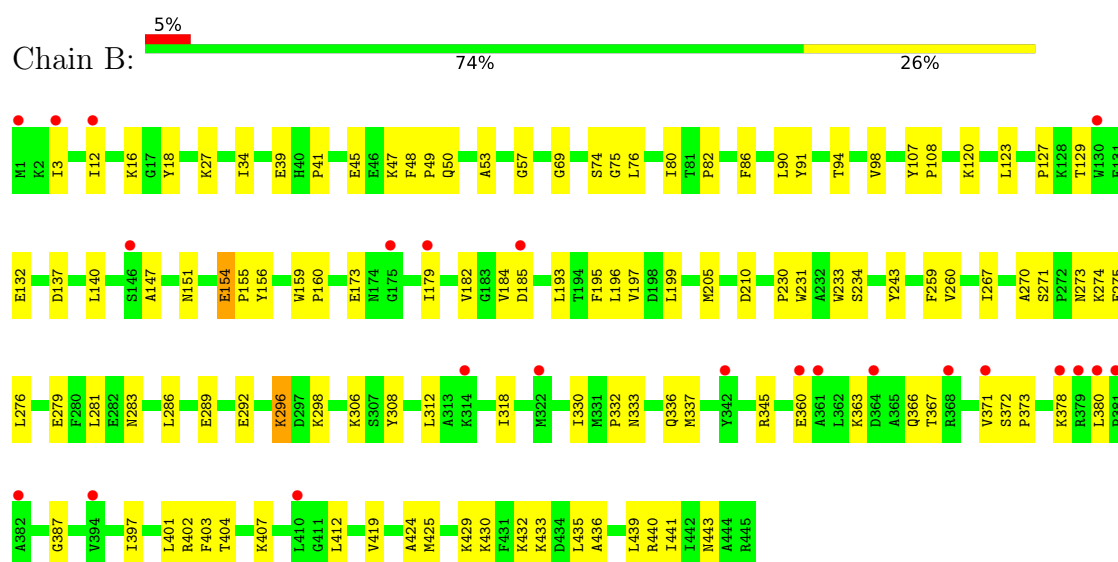
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Extracellular solute-binding protein family 1, viral genome protein



- Molecule 1: Extracellular solute-binding protein family 1, viral genome protein



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  50% 50%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.30Å 81.42Å 77.19Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	48.29 – 2.05 48.29 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.29-2.05) 88.9 (48.29-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.221 , 0.254 (Not available) , 0.243	Depositor DCC
R_{free} test set	1912 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/3505	0.74	4/4749 (0.1%)
1	B	0.32	0/3534	0.75	2/4786 (0.0%)
All	All	0.31	0/7039	0.75	6/9535 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	GLU	CA-C-N	5.74	125.60	119.28
1	B	154	GLU	C-N-CA	5.74	125.60	119.28
1	A	174	ASN	CB-CA-C	-5.23	110.11	117.23
1	A	154	GLU	CA-C-N	5.21	124.87	119.56
1	A	154	GLU	C-N-CA	5.21	124.87	119.56
1	A	133	ILE	CB-CA-C	-5.08	108.96	114.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3425	0	3464	132	0
1	B	3454	0	3504	117	0
2	C	23	22	21	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	23	22	21	3	0
3	A	154	0	0	16	2
3	B	219	0	0	13	1
All	All	7298	44	7010	236	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:HB2	3:B:601:HOH:O	1.34	1.23
1:A:226:THR:C	3:A:601:HOH:O	1.84	1.18
1:B:151:ASN:ND2	3:B:601:HOH:O	1.84	1.10
1:B:185:ASP:HB2	1:B:366:GLN:HG3	1.36	1.08
1:A:185:ASP:HB2	1:A:366:GLN:HG3	1.11	1.05
1:B:306:LYS:NZ	3:B:602:HOH:O	1.88	1.04
1:A:227:ILE:HG13	3:A:601:HOH:O	1.67	0.93
1:B:185:ASP:CB	1:B:366:GLN:HG3	2.03	0.89
1:B:205:MET:SD	3:B:808:HOH:O	2.32	0.88
1:A:6:GLY:H	1:A:273:ASN:HD21	1.24	0.86
1:B:151:ASN:CB	3:B:601:HOH:O	2.00	0.86
1:A:226:THR:O	3:A:601:HOH:O	1.80	0.86
1:B:185:ASP:HB2	1:B:366:GLN:CG	2.08	0.83
1:B:360:GLU:OE1	3:B:603:HOH:O	1.95	0.83
1:A:332:PRO:HB2	1:A:337:MET:HE3	1.61	0.82
1:A:254:GLN:O	3:A:602:HOH:O	1.96	0.81
1:A:90:LEU:HD23	1:A:108:PRO:HG2	1.62	0.81
1:B:34:ILE:HD13	1:B:276:LEU:HD22	1.63	0.80
1:A:190:LYS:O	1:A:194:THR:HG23	1.81	0.79
1:A:155:PRO:HG3	1:A:345:ARG:HA	1.63	0.79
1:A:248:LEU:HB2	1:A:256:SER:OG	1.82	0.79
1:A:46:GLU:OE2	3:A:605:HOH:O	2.01	0.79
1:A:6:GLY:H	1:A:273:ASN:ND2	1.81	0.78
1:A:165:ASP:O	3:A:604:HOH:O	2.01	0.78
1:A:164:ALA:O	3:A:603:HOH:O	2.01	0.78
1:B:90:LEU:HD23	1:B:108:PRO:HG2	1.67	0.76
1:B:279:GLU:OE2	1:B:283:ASN:ND2	2.17	0.76
1:A:185:ASP:CB	1:A:366:GLN:HG3	2.05	0.76
1:A:327:LYS:NZ	3:A:608:HOH:O	2.18	0.74
1:A:185:ASP:HB2	1:A:366:GLN:CG	2.07	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:CD2	1:B:281:LEU:HD13	2.22	0.74
1:B:27:LYS:NZ	1:B:289:GLU:OE2	2.22	0.73
1:B:155:PRO:HG3	1:B:345:ARG:HA	1.72	0.72
1:A:129:THR:HA	1:A:250:THR:HG22	1.70	0.71
1:B:366:GLN:NE2	3:B:605:HOH:O	2.22	0.71
1:B:276:LEU:HG	3:B:636:HOH:O	1.91	0.70
1:B:332:PRO:HB2	1:B:337:MET:HE3	1.74	0.70
1:B:179:ILE:HD12	1:B:179:ILE:H	1.57	0.70
1:B:69:GLY:HA3	1:B:333:ASN:O	1.93	0.69
1:A:435:LEU:HD22	1:B:435:LEU:HD12	1.74	0.68
1:B:156:TYR:HB2	2:D:1:GLC:H62	1.76	0.67
1:A:439:LEU:HD11	1:B:425:MET:HG3	1.75	0.67
1:A:184:VAL:HB	1:A:366:GLN:HG2	1.76	0.67
1:B:12:ILE:HD11	1:B:16:LYS:CB	2.24	0.67
1:A:336:GLN:HA	1:A:374:PHE:CD2	2.29	0.67
1:B:182:VAL:O	1:B:366:GLN:NE2	2.23	0.67
1:A:158:THR:HG23	1:A:196:LEU:HD22	1.76	0.67
1:A:34:ILE:HD13	1:A:276:LEU:HD13	1.78	0.66
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.31	0.66
1:A:112:GLU:OE2	2:C:1:GLC:O2	2.05	0.66
1:A:182:VAL:O	1:A:366:GLN:NE2	2.28	0.66
1:B:332:PRO:HB2	1:B:337:MET:CE	2.26	0.66
1:A:129:THR:HG22	1:A:250:THR:CG2	2.26	0.66
1:A:248:LEU:CB	1:A:256:SER:OG	2.44	0.66
1:B:308:TYR:CE2	1:B:312:LEU:HD11	2.31	0.65
1:A:436:ALA:HA	1:B:432:LYS:HZ1	1.62	0.65
1:B:140:LEU:HD12	1:B:147:ALA:HA	1.79	0.65
1:A:216:ALA:HB1	1:A:220:LYS:NZ	2.12	0.64
1:A:34:ILE:CD1	1:A:276:LEU:HD22	2.29	0.63
1:A:69:GLY:HA3	1:A:333:ASN:O	1.98	0.63
1:A:251:PHE:O	3:A:602:HOH:O	2.15	0.63
1:B:234:SER:HB2	1:B:298:LYS:HD3	1.81	0.63
1:A:339:ALA:HB2	1:A:374:PHE:HE2	1.64	0.63
1:B:184:VAL:HB	1:B:366:GLN:HG2	1.81	0.62
1:A:27:LYS:HD3	3:A:661:HOH:O	1.98	0.62
1:B:184:VAL:H	1:B:366:GLN:HE21	1.46	0.62
1:A:254:GLN:HB2	3:A:602:HOH:O	1.98	0.61
1:A:34:ILE:HD13	1:A:276:LEU:CD1	2.30	0.61
1:A:267:ILE:HG21	1:A:274:LYS:HG3	1.83	0.61
1:B:12:ILE:HD11	1:B:16:LYS:HB3	1.83	0.60
1:B:182:VAL:C	1:B:366:GLN:HE22	2.09	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:MET:O	1:A:326:GLN:HG2	2.02	0.59
1:A:34:ILE:CD1	1:A:276:LEU:CD2	2.81	0.59
1:A:425:MET:HE1	1:B:443:ASN:OD1	2.03	0.59
1:B:231:TRP:O	1:B:298:LYS:HD2	2.03	0.59
1:A:198:ASP:HA	1:A:201:LYS:HG2	1.85	0.58
1:A:21:LEU:O	1:A:24:VAL:HG22	2.02	0.58
1:B:173:GLU:OE1	3:B:604:HOH:O	2.16	0.58
1:A:129:THR:OG1	1:A:132:GLU:HG3	2.04	0.58
1:A:312:LEU:C	1:A:314:LYS:H	2.12	0.57
1:B:234:SER:CB	1:B:298:LYS:HD3	2.34	0.57
1:A:256:SER:N	3:A:606:HOH:O	2.09	0.57
1:B:184:VAL:N	1:B:366:GLN:HE21	2.02	0.57
1:A:155:PRO:HD3	1:A:345:ARG:HG3	1.85	0.57
1:A:32:THR:HG21	1:A:34:ILE:HD12	1.87	0.56
1:A:443:ASN:OD1	1:B:425:MET:HE1	2.05	0.56
1:A:32:THR:CG2	1:A:34:ILE:HD12	2.35	0.56
1:A:109:ILE:CD1	1:A:286:LEU:HD11	2.35	0.56
1:A:6:GLY:N	1:A:273:ASN:HD21	1.99	0.56
1:A:193:LEU:HD23	1:A:358:VAL:HG13	1.89	0.55
1:B:53:ALA:HA	1:B:270:ALA:HB3	1.87	0.55
1:A:98:VAL:CG2	1:A:106:ALA:HB3	2.37	0.55
1:A:339:ALA:CB	1:A:374:PHE:HE2	2.20	0.55
1:A:98:VAL:HG21	1:A:106:ALA:HB3	1.89	0.55
1:A:206:ASN:OD1	1:A:208:ASP:HB2	2.07	0.55
1:B:419:VAL:HG21	1:B:424:ALA:HB2	1.88	0.54
1:B:234:SER:HB2	1:B:298:LYS:CD	2.37	0.54
1:B:123:LEU:HD21	1:B:127:PRO:HD3	1.90	0.54
1:B:12:ILE:CD1	1:B:16:LYS:HB2	2.37	0.53
1:A:384:LEU:HD13	1:A:393:MET:HG2	1.90	0.53
1:B:185:ASP:HB2	1:B:366:GLN:CD	2.34	0.53
1:A:312:LEU:O	1:A:318:ILE:HD12	2.09	0.53
1:A:129:THR:HG22	1:A:250:THR:HG22	1.90	0.52
1:B:372:SER:OG	1:B:373:PRO:HD3	2.09	0.52
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.43	0.52
1:A:439:LEU:HD22	1:B:432:LYS:HE2	1.92	0.52
1:A:341:TRP:CD1	2:C:2:GLC:H4	2.45	0.52
1:B:12:ILE:CD1	1:B:16:LYS:CB	2.87	0.52
1:A:68:PHE:HD2	1:A:77:LEU:HD11	1.74	0.52
1:B:367:THR:O	1:B:371:VAL:HG23	2.10	0.52
1:A:234:SER:HB3	1:A:298:LYS:HD3	1.91	0.52
1:B:137:ASP:HA	1:B:147:ALA:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:CD1	1:B:147:ALA:HA	2.40	0.51
1:A:130:TRP:CD1	1:A:249:PRO:HB2	2.45	0.51
1:A:367:THR:O	1:A:371:VAL:HG23	2.10	0.51
1:B:156:TYR:HB2	2:D:1:GLC:C6	2.41	0.51
1:A:155:PRO:HG3	1:A:345:ARG:CA	2.37	0.51
1:B:234:SER:HB2	1:B:298:LYS:NZ	2.26	0.50
1:A:254:GLN:C	3:A:602:HOH:O	2.48	0.50
1:A:339:ALA:HB2	1:A:374:PHE:CE2	2.46	0.50
1:B:182:VAL:C	1:B:366:GLN:NE2	2.69	0.50
1:A:34:ILE:HD12	1:A:276:LEU:HD22	1.95	0.49
1:A:365:ALA:O	1:A:369:ILE:HG13	2.12	0.49
1:A:425:MET:HE1	1:B:443:ASN:CG	2.37	0.49
1:B:48:PHE:N	1:B:49:PRO:HD2	2.28	0.49
1:A:273:ASN:HB3	1:A:276:LEU:HD12	1.94	0.48
1:A:234:SER:CB	1:A:298:LYS:HD3	2.43	0.48
1:A:171:LYS:HB3	1:A:178:ASP:HB3	1.94	0.48
1:A:332:PRO:HB2	1:A:337:MET:CE	2.38	0.48
1:B:433:LYS:HB2	1:B:433:LYS:HE3	1.57	0.48
1:A:387:GLY:HA2	1:A:412:LEU:HD13	1.94	0.48
1:A:138:LYS:HE2	1:A:204:HIS:HE1	1.78	0.48
1:B:436:ALA:O	1:B:440:ARG:HG3	2.14	0.48
1:B:425:MET:O	1:B:429:LYS:HD3	2.14	0.48
1:B:80:ILE:HG22	1:B:82:PRO:HD3	1.95	0.47
1:A:431:PHE:CE1	1:B:403:PHE:HB3	2.49	0.47
1:A:432:LYS:HE3	3:B:708:HOH:O	2.13	0.47
1:A:278:LYS:HE2	3:A:614:HOH:O	2.14	0.47
1:B:151:ASN:HB3	1:B:210:ASP:C	2.39	0.47
1:B:179:ILE:HG23	1:B:336:GLN:HG2	1.95	0.47
1:B:195:PHE:O	1:B:199:LEU:HG	2.15	0.47
1:B:275:GLU:CD	1:B:275:GLU:H	2.23	0.47
1:B:306:LYS:NZ	3:B:619:HOH:O	2.44	0.47
1:A:371:VAL:HG12	1:A:371:VAL:O	2.15	0.47
1:A:419:VAL:HG21	1:A:424:ALA:HB2	1.97	0.46
1:A:86:PHE:HZ	1:A:286:LEU:HD22	1.80	0.46
1:A:336:GLN:HG3	1:A:374:PHE:HB2	1.98	0.46
1:A:439:LEU:CD1	1:B:425:MET:HG3	2.43	0.46
1:B:154:GLU:HA	1:B:155:PRO:HD3	1.80	0.46
1:A:393:MET:HE3	1:A:393:MET:HB2	1.84	0.46
1:B:419:VAL:CG2	1:B:424:ALA:HB2	2.45	0.46
1:B:129:THR:OG1	1:B:132:GLU:HG3	2.16	0.46
1:B:273:ASN:HB3	1:B:276:LEU:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LYS:HE3	1:B:407:LYS:HB2	1.83	0.45
1:A:129:THR:CA	1:A:250:THR:HG22	2.42	0.45
1:A:350:ASN:ND2	1:A:355:ARG:HD2	2.31	0.45
1:B:260:VAL:O	1:B:330:ILE:HD12	2.16	0.45
1:A:78:ALA:HB1	1:A:274:LYS:HD3	1.98	0.45
1:A:393:MET:HE2	1:B:404:THR:CG2	2.46	0.45
1:B:292:GLU:O	1:B:296:LYS:HB2	2.17	0.45
1:B:312:LEU:O	1:B:318:ILE:HD12	2.17	0.45
1:B:98:VAL:HG21	1:B:108:PRO:HD3	1.99	0.45
1:B:397:ILE:O	1:B:401:LEU:HG	2.17	0.45
1:A:53:ALA:HA	1:A:270:ALA:HB3	1.98	0.45
1:A:129:THR:HA	1:A:250:THR:H	1.81	0.45
1:B:274:LYS:HB2	1:B:274:LYS:HE3	1.75	0.45
1:A:34:ILE:HD13	1:A:276:LEU:CD2	2.48	0.44
1:B:107:TYR:HD2	1:B:281:LEU:HD13	1.77	0.44
1:A:98:VAL:O	1:A:98:VAL:HG22	2.17	0.44
1:A:216:ALA:HB1	1:A:220:LYS:HZ1	1.79	0.44
1:A:384:LEU:CD1	1:A:393:MET:HG2	2.47	0.44
1:B:120:LYS:HE3	1:B:243:TYR:O	2.17	0.44
1:B:185:ASP:CA	1:B:366:GLN:HG3	2.47	0.44
1:B:430:LYS:C	1:B:430:LYS:HD2	2.43	0.44
1:A:281:LEU:O	1:A:286:LEU:HD13	2.18	0.44
1:A:91:TYR:HA	1:A:92:PRO:HD3	1.90	0.44
1:A:137:ASP:HA	1:A:147:ALA:HB2	2.00	0.44
1:B:159:TRP:N	1:B:160:PRO:CD	2.80	0.44
1:A:184:VAL:H	1:A:366:GLN:HE21	1.64	0.43
1:A:314:LYS:HE3	1:A:314:LYS:HB2	1.82	0.43
1:A:48:PHE:N	1:A:49:PRO:HD2	2.33	0.43
1:A:110:ALA:HA	1:A:303:VAL:HA	2.00	0.43
1:A:397:ILE:O	1:A:401:LEU:HG	2.18	0.43
1:B:179:ILE:HD12	1:B:179:ILE:N	2.28	0.43
1:B:193:LEU:O	1:B:197:VAL:HG23	2.19	0.43
1:B:12:ILE:HG12	1:B:16:LYS:HB2	2.00	0.43
1:B:155:PRO:HG3	1:B:345:ARG:CA	2.44	0.43
1:A:29:GLU:OE2	1:A:35:LYS:HG2	2.19	0.43
1:A:239:SER:O	1:A:240:LYS:HB2	2.19	0.43
1:A:166:GLY:O	1:A:186:ASN:ND2	2.52	0.43
1:A:315:ASP:OD1	1:A:317:ARG:N	2.45	0.43
1:A:380:LEU:HG	1:B:380:LEU:CD1	2.49	0.43
1:B:47:LYS:O	1:B:50:GLN:HB3	2.19	0.43
1:A:128:LYS:O	1:A:250:THR:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ALA:CA	1:B:432:LYS:HZ1	2.30	0.42
1:B:185:ASP:N	1:B:366:GLN:HG3	2.34	0.42
1:A:27:LYS:HB2	1:A:27:LYS:HE3	1.69	0.42
1:B:39:GLU:C	1:B:41:PRO:HD3	2.45	0.42
1:A:345:ARG:HB3	1:A:345:ARG:HH11	1.83	0.42
1:B:12:ILE:HG21	1:B:18:TYR:HB3	2.00	0.42
1:A:424:ALA:O	1:A:428:ILE:HG13	2.20	0.42
1:B:260:VAL:HB	1:B:330:ILE:HA	2.01	0.42
1:A:285:LEU:HG	1:A:286:LEU:HD12	2.01	0.42
1:A:336:GLN:HA	1:A:374:PHE:CE2	2.54	0.42
1:B:371:VAL:HG12	1:B:371:VAL:O	2.20	0.42
1:A:425:MET:HG3	1:B:439:LEU:HD11	2.01	0.42
1:B:91:TYR:O	1:B:94:THR:OG1	2.28	0.42
1:B:196:LEU:HA	1:B:199:LEU:HD12	2.01	0.42
1:B:332:PRO:HB2	1:B:337:MET:HE1	2.01	0.42
1:B:3:ILE:HG23	1:B:57:GLY:O	2.19	0.42
1:B:75:GLY:O	1:B:441:ILE:HG23	2.19	0.42
1:B:271:SER:O	1:B:274:LYS:HE3	2.20	0.42
1:A:5:GLU:HA	1:A:273:ASN:HD21	1.84	0.42
1:B:402:ARG:NH2	3:B:628:HOH:O	2.52	0.42
1:B:179:ILE:CG2	1:B:336:GLN:HG2	2.49	0.42
1:A:227:ILE:CG1	3:A:601:HOH:O	2.43	0.42
1:B:156:TYR:CB	2:D:1:GLC:H62	2.48	0.42
1:B:267:ILE:HG21	1:B:274:LYS:HG3	2.02	0.41
1:A:23:GLU:HG3	3:A:689:HOH:O	2.21	0.41
1:B:12:ILE:CG2	1:B:18:TYR:HB3	2.50	0.41
1:A:44:LEU:HD12	1:A:44:LEU:C	2.46	0.41
1:B:372:SER:N	1:B:373:PRO:CD	2.84	0.41
1:B:387:GLY:HA2	1:B:412:LEU:HD13	2.03	0.41
1:B:363:LYS:CE	3:B:603:HOH:O	2.69	0.41
1:B:378:LYS:HD2	1:B:378:LYS:HA	1.79	0.41
1:B:74:SER:HB2	1:B:76:LEU:HG	2.02	0.41
1:B:45:GLU:OE1	1:B:45:GLU:N	2.46	0.40
1:A:360:GLU:O	1:A:364:ASP:HB2	2.22	0.40
1:A:86:PHE:O	1:A:89:LYS:HB2	2.21	0.40
1:A:99:ARG:NH1	1:A:104:LEU:HD21	2.36	0.40
1:A:119:ASN:CG	1:A:122:LEU:HD13	2.46	0.40
1:A:259:PHE:CD1	1:A:331:MET:HG2	2.56	0.40
1:B:86:PHE:HZ	1:B:286:LEU:CD1	2.34	0.40
1:A:274:LYS:HE3	1:A:274:LYS:HB2	1.95	0.40
1:A:247:VAL:HA	1:A:324:ASN:HD21	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:SER:HA	1:A:373:PRO:HD3	1.74	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:697:HOH:O	3:B:696:HOH:O[2_746]	1.91	0.29
3:A:667:HOH:O	3:A:693:HOH:O[2_855]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/445 (89%)	385 (97%)	11 (3%)	0	100	100
1	B	398/445 (89%)	393 (99%)	5 (1%)	0	100	100
All	All	794/890 (89%)	778 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/356 (99%)	349 (99%)	3 (1%)	70	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	356/356 (100%)	354 (99%)	2 (1%)	78	83
All	All	708/712 (99%)	703 (99%)	5 (1%)	76	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	259	PHE
1	A	393	MET
1	B	259	PHE
1	B	296	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	204	HIS
1	A	254	GLN
1	A	273	ASN
1	A	326	GLN
1	A	350	ASN
1	B	235	ASN
1	B	366	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	C	1	2	12,12,12	1.78	4 (33%)	17,17,17	1.08	2 (11%)
2	GLC	C	2	2	11,11,12	1.66	2 (18%)	15,15,17	1.30	2 (13%)
2	GLC	D	1	2	12,12,12	0.48	0	17,17,17	2.14	5 (29%)
2	GLC	D	2	2	11,11,12	0.72	0	15,15,17	2.35	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLC	C2-C3	3.23	1.57	1.52
2	C	2	GLC	C4-C5	3.07	1.59	1.53
2	C	1	GLC	O4-C4	2.86	1.50	1.43
2	C	1	GLC	C1-C2	2.77	1.58	1.52
2	C	1	GLC	C3-C2	2.72	1.59	1.52
2	C	1	GLC	C4-C5	2.45	1.58	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	6.78	121.28	112.19
2	D	1	GLC	O4-C4-C5	4.89	121.36	109.32
2	D	1	GLC	C4-C3-C2	-4.73	102.53	110.83
2	D	2	GLC	O5-C1-C2	3.29	118.65	110.79
2	D	2	GLC	C1-C2-C3	2.96	113.96	109.64
2	D	1	GLC	C1-O5-C5	2.88	119.22	113.65
2	D	1	GLC	O5-C1-C2	2.76	115.15	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C3-C4-C5	-2.72	105.30	110.23
2	C	2	GLC	C1-O5-C5	2.54	115.59	112.19
2	C	2	GLC	C2-C3-C4	-2.47	106.51	110.86
2	D	1	GLC	O5-C5-C4	-2.41	105.35	109.70
2	C	1	GLC	C4-C3-C2	-2.32	106.77	110.83
2	C	1	GLC	O5-C5-C6	2.08	111.61	106.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

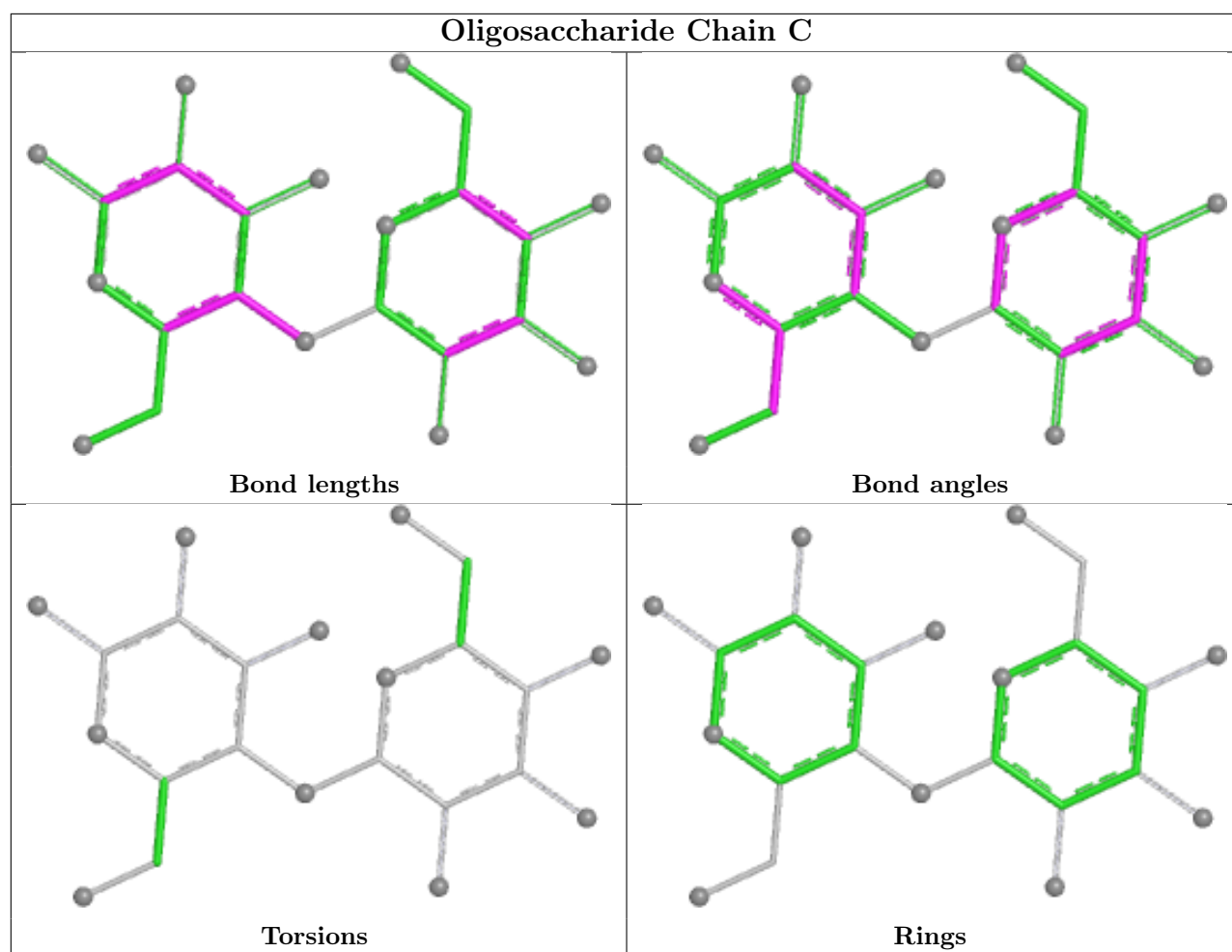
Mol	Chain	Res	Type	Atoms
2	D	2	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6

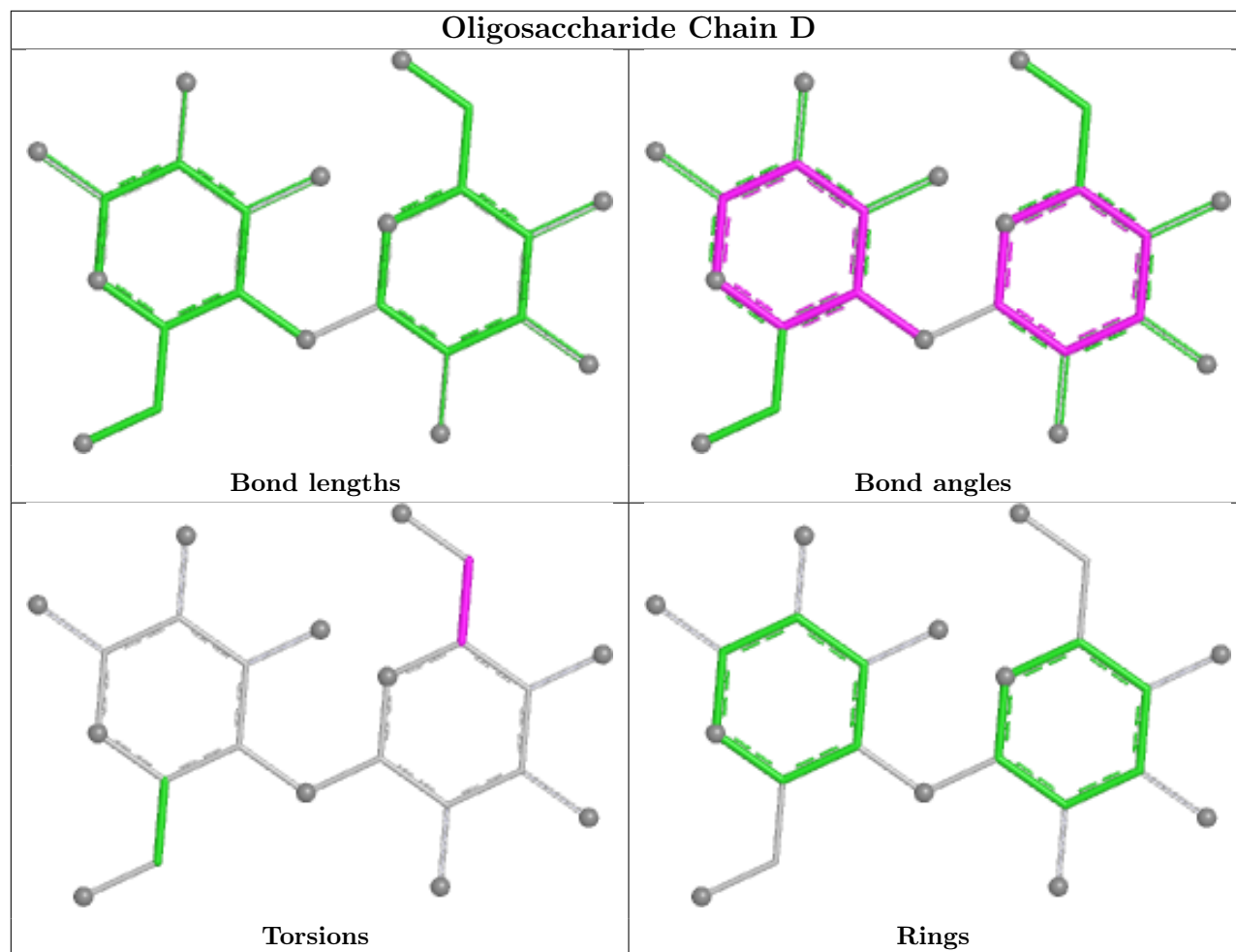
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLC	3	0
2	C	1	GLC	1	0
2	C	2	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/445 (99%)	1.17	78 (17%) 4 3	26, 41, 62, 104	0
1	B	445/445 (100%)	0.61	23 (5%) 33 33	24, 33, 47, 68	0
All	All	887/890 (99%)	0.89	101 (11%) 10 9	24, 37, 57, 104	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	PHE	6.1
1	A	355	ARG	4.7
1	A	375	GLY	4.6
1	A	184	VAL	3.6
1	B	314	LYS	3.6
1	A	164	ALA	3.4
1	A	444	ALA	3.3
1	B	179	ILE	3.3
1	B	410	LEU	3.3
1	B	342	TYR	3.2
1	A	376	GLY	3.2
1	B	382	ALA	3.2
1	A	337	MET	3.1
1	A	130	TRP	3.1
1	A	50	GLN	3.1
1	B	381	PRO	3.1
1	A	208	ASP	3.1
1	A	373	PRO	3.1
1	A	328	GLY	3.0
1	A	332	PRO	3.0
1	B	1	MET	3.0
1	A	270	ALA	3.0
1	A	4	GLU	3.0
1	A	197	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	ILE	3.0
1	B	130	TRP	2.9
1	A	330	ILE	2.8
1	B	322	MET	2.8
1	B	361	ALA	2.8
1	B	12	ILE	2.8
1	A	351	ALA	2.8
1	A	83	ASP	2.8
1	B	364	ASP	2.8
1	A	24	VAL	2.8
1	A	331	MET	2.7
1	A	182	VAL	2.7
1	A	312	LEU	2.7
1	A	124	PRO	2.7
1	A	23	GLU	2.7
1	A	102	GLY	2.7
1	A	237	ASP	2.7
1	A	350	ASN	2.6
1	B	3	ILE	2.6
1	B	380	LEU	2.6
1	A	342	TYR	2.6
1	A	66	ASP	2.6
1	A	191	ALA	2.6
1	A	90	LEU	2.6
1	A	173	GLU	2.5
1	B	378	LYS	2.5
1	A	94	THR	2.5
1	A	338	SER	2.5
1	B	394	VAL	2.5
1	A	308	TYR	2.5
1	B	360	GLU	2.5
1	A	212	SER	2.5
1	A	358	VAL	2.4
1	A	382	ALA	2.4
1	A	278	LYS	2.4
1	A	166	GLY	2.4
1	A	93	PHE	2.4
1	A	367	THR	2.4
1	A	313	ALA	2.4
1	A	300	LEU	2.4
1	B	175	GLY	2.4
1	B	185	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	125	ASN	2.3
1	A	286	LEU	2.3
1	A	251	PHE	2.3
1	A	369	ILE	2.3
1	A	127	PRO	2.3
1	A	347	ALA	2.3
1	A	372	SER	2.3
1	A	149	MET	2.3
1	A	340	PHE	2.3
1	A	185	ASP	2.3
1	A	88	ASP	2.2
1	A	326	GLN	2.2
1	A	177	TYR	2.2
1	A	314	LYS	2.2
1	A	242	ASN	2.2
1	A	165	ASP	2.2
1	B	368	ARG	2.2
1	A	172	TYR	2.2
1	A	7	LYS	2.2
1	A	305	LEU	2.1
1	A	256	SER	2.1
1	A	128	LYS	2.1
1	A	307	SER	2.1
1	B	146	SER	2.1
1	A	5	GLU	2.1
1	A	170	PHE	2.1
1	A	195	PHE	2.1
1	B	371	VAL	2.1
1	A	85	ALA	2.1
1	A	295	ASN	2.0
1	A	364	ASP	2.0
1	A	335	PRO	2.0
1	A	371	VAL	2.0
1	B	379	ARG	2.0
1	A	301	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

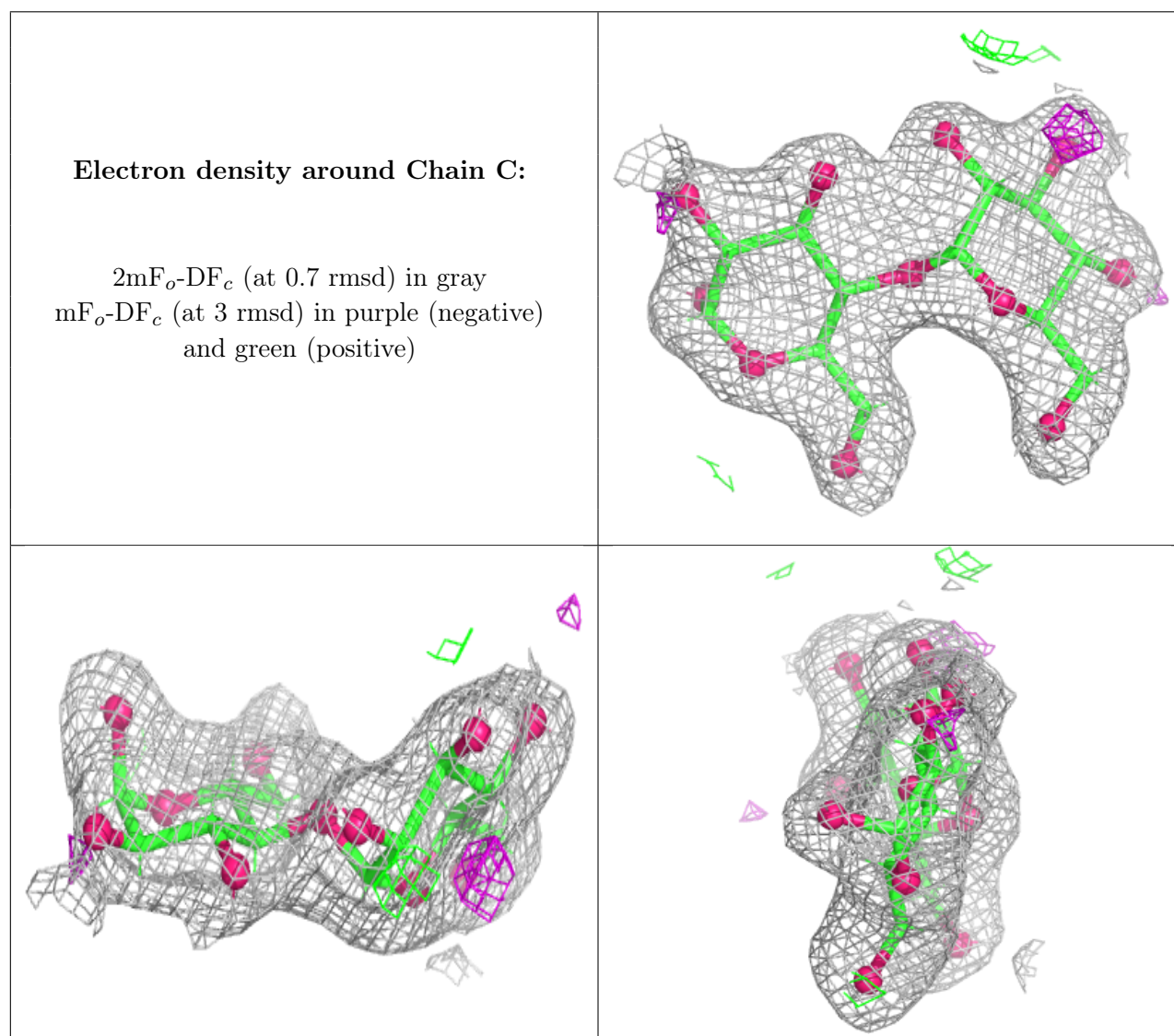
There are no non-standard protein/DNA/RNA residues in this entry.

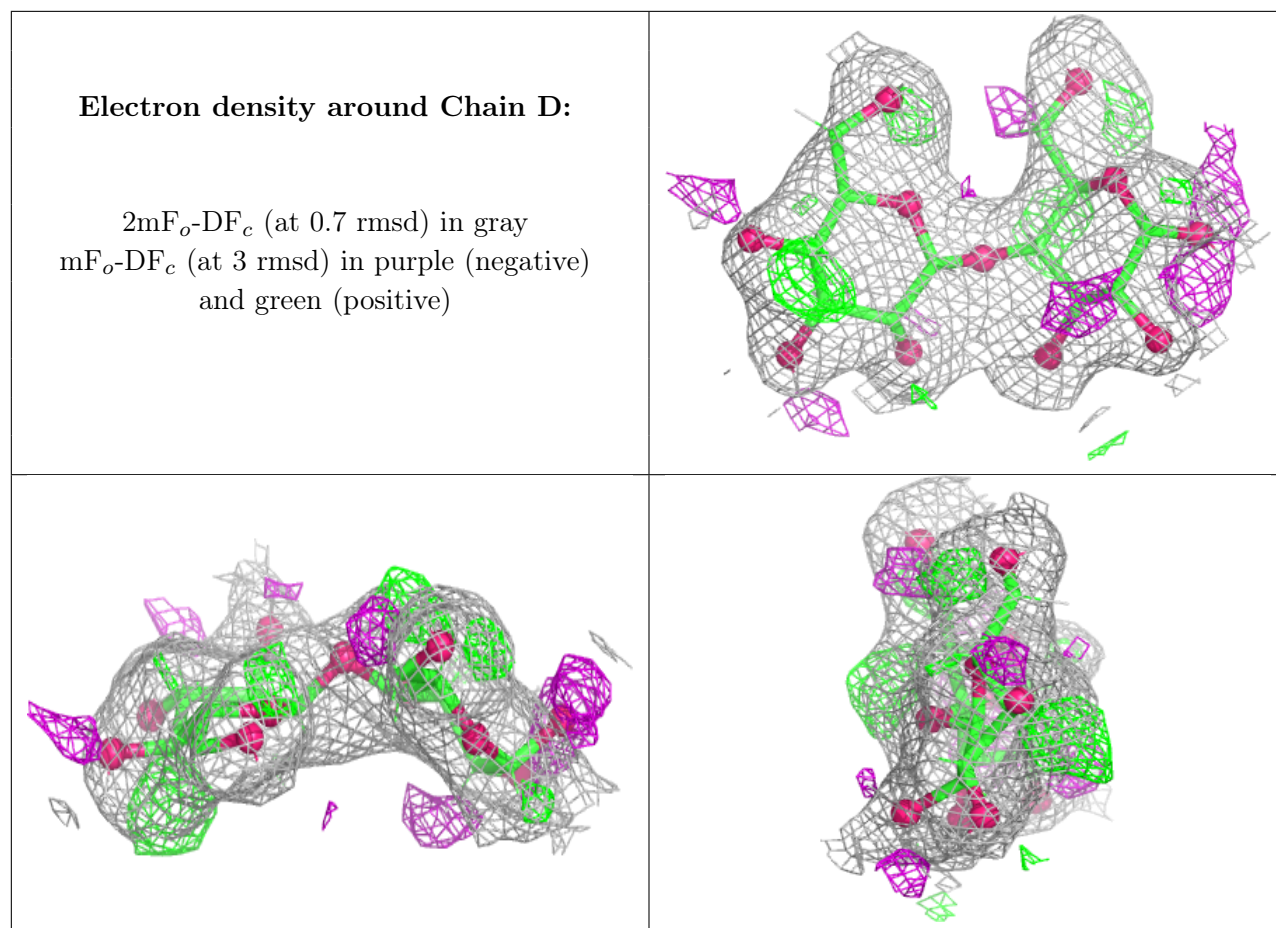
6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	D	1	12/12	0.78	0.17	31,38,54,62	0
2	GLC	D	2	11/12	0.80	0.14	28,41,51,55	0
2	GLC	C	1	12/12	0.90	0.09	33,41,49,50	0
2	GLC	C	2	11/12	0.93	0.09	36,49,64,77	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.